Nano phase diagrams: 3D phase diagrams of two-component nanoparticles – effects of size, average composition and temperature

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Determining binary phase diagrams for nanoparticles proves to be a very difficult task regardless if it is tried either by computer simulations, theoretical considerations or experiments. In this work, using 3D Object Stochastic Kinetic Modelling Framework (3DO-SKMF) computer simulations, we reveal some of the reasons why this is the case. First of all, even the expressions "phase diagram" and "phase composition" are usually not well-defined. We show the two different types of phase diagrams that are rarely distinguished. For phase separating nanoparticles, one diagram shows the equilibrium phase compositions in two-phase state while the other represents if the system is in an alloyed or in a separated state. We calculate both diagrams for the case of binary Janus nanoparticles and show their dependences on size and average composition. The equilibrium compositions of the phases change with both the size and the average composition of the particle. This means that the use of 3D phase diagrams is unavoidable even if the size of the particle is fixed. The careful investigation of the simulation results reveals the essential role that the interfaces play in the behaviour of the system hence in the shape of the phase diagrams. We also point out that the methods used to determine the phase compositions in nanoparticles have a substantial influence on the details of both experimentally and theoretically constructed phase diagrams.

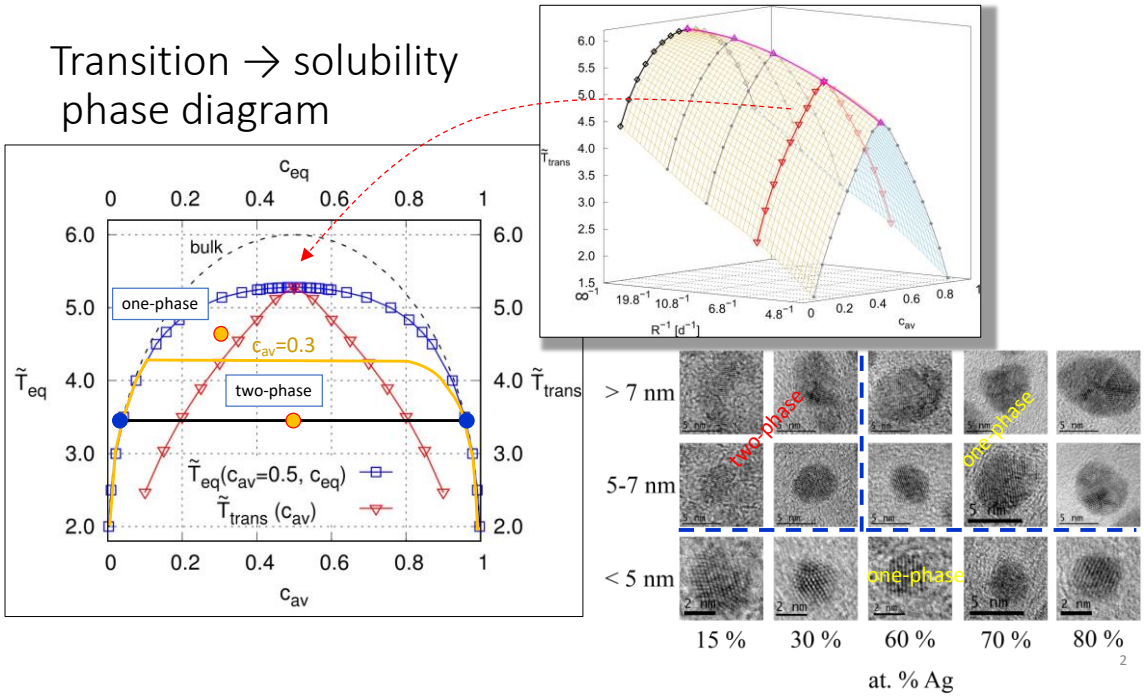

Figure 1: Nano phase diagrams – theoretical and experimental (Ag-Cu nanoparticles) results [1,2]

References

[1] A. Taranovskyy, J.J. Tomán; B.D. Gajdics, Z. Erdélyi, *3D phase diagrams and the thermal stability of two-component Janus nanoparticles: effects of size, average composition and temperature*. Physical Chemistry Chemical Physics **23** pp. 6116-6127 (2021)

[2] G., Radnóczi ; E., Bokányi ; Z., Erdélyi ; F., Misják, *Size dependent spinodal decomposition in Cu-Ag nanoparticles.* Acta Materialia **123** pp. 82-89. (2017)